Introduction to Neural Networks 2

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Talk Overview

1. Backpropagation in Neural Networks

Outline

HOW TO TRAIN A NEURAL NET?

- Put in training inputs, get the output
- Compare output to correct answers: look at loss function J
- Adjust and repeat!
- Backpropagation tells us how to make a single adjustment using calculus.

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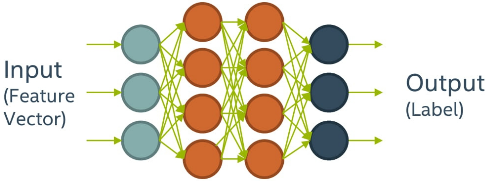

HOW HAVE WE TRAINED BEFORE?

Gradient Descent!

1. Make prediction
2. Calculate Loss
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4. Update parameters by taking a step in the opposite direction
5. Iterate

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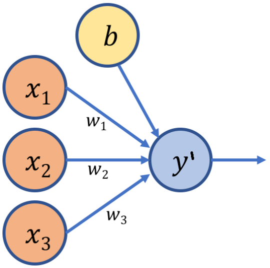
Logistic Regression as Neural Network (Refresher 1/5)

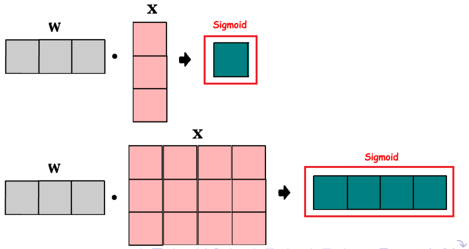


Feedforwad one sample

1. $z = \mathbf{w}^T \cdot \mathbf{x} + b$
2. $y = \sigma(z)$

Feedforwad batch

1. $\mathbf{z} = \mathbf{w} \cdot \mathbf{X} + b$
2. $\mathbf{y} = \sigma(\mathbf{z})$



Logistic Regression as Neural Network (Refresher 2/5)

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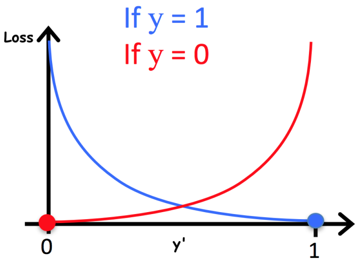
  - if y = 0 : Loss = -log(1-y')



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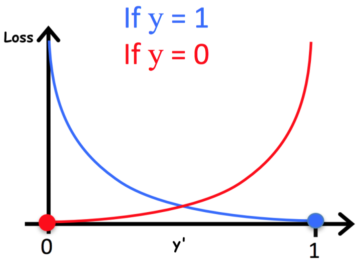

Loss$= \ell =$ -ylog(y')-(1-y)log(1-y')

Logistic Regression as Neural Network (Refresher 3/5)

- For n features: $z = \sum_{i=0}^{i=n} w_i x_i$, (w_0 is the bias)
- vector representation $z = \mathbf{w}^T\mathbf{x}$
- $y = sigmoid(z) = \sigma(z)$
- $\ell = -ylog(y') - (1-y)log(1-y')$

Logistic Regression as Neural Network (Refresher 4/5)

$$
\begin{aligned}
\frac{d\ell}{dw_i} &= \frac{d\ell}{dy'}\frac{dy'}{dw_i} = \frac{d\ell}{dy'}\frac{dy'}{dz}\frac{dz}{dw_i} \\
&= \underbrace{\Big[\frac{-y}{\sigma(z)} + \frac{1-y}{1-\sigma(z)}\Big]}_{\frac{d\ell}{dy'}} * \underbrace{\sigma(z)(1-\sigma(z))}_{\frac{dy'}{dz}} * \underbrace{x_i}_{\frac{dz}{dw_i}} \\
&= \underbrace{\Big[\frac{-y(1-\sigma(z)) + (1-y)\sigma(z)}{\sigma(z)(1-\sigma(z))}\Big]}_{\frac{d\ell}{dy'}} * \underbrace{\sigma(z)(1-\sigma(z))}_{\frac{dy'}{dz}} * \underbrace{x_i}_{\frac{dz}{dw_i}} \\
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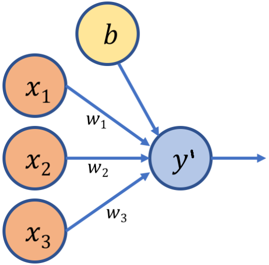
&= (\sigma(z) - y) * x_i \\
&= (y' - y) * x_i
\end{aligned}
$$

Logistic Regression as Neural Network (Refresher 5/5)

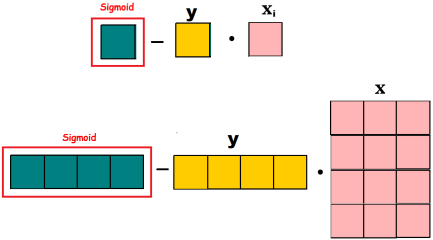


Loss one sample (using log loss)

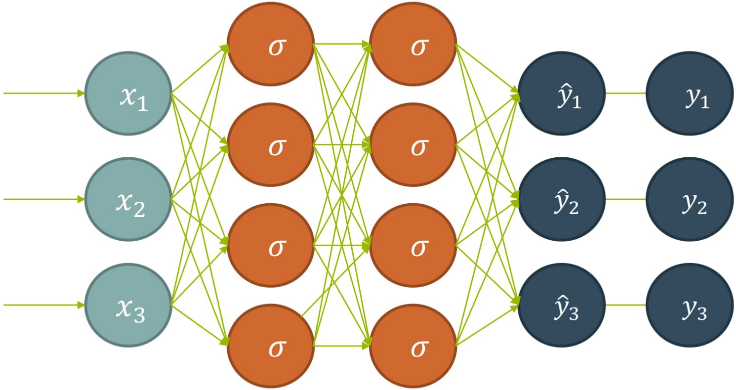
1. $\frac{d\ell}{dw_i} = (y' - y) * x_i$

Loss four samples (using log loss)

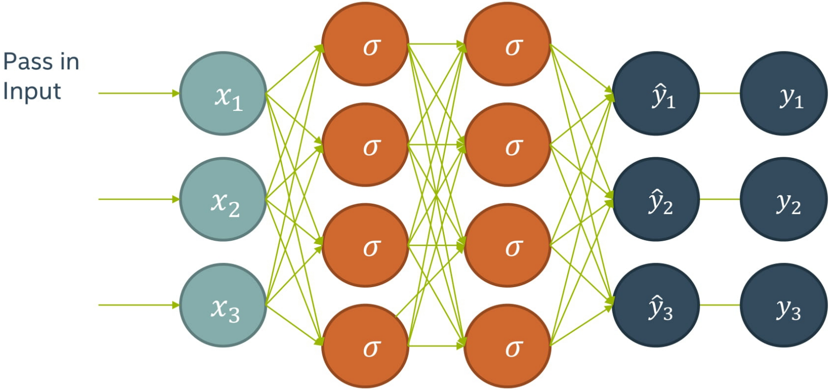
1. $\frac{d\ell}{d\mathbf{w}} = (\mathbf{y}' - \mathbf{y}) \cdot \mathbf{X}^T$



FEEDFORWARD NEURAL NETWORK

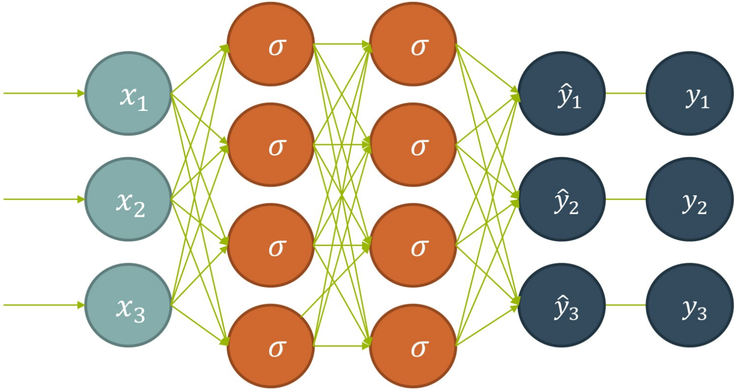


FORWARD PROPAGATION



FORWARD PROPAGATION

Calculate each Layer



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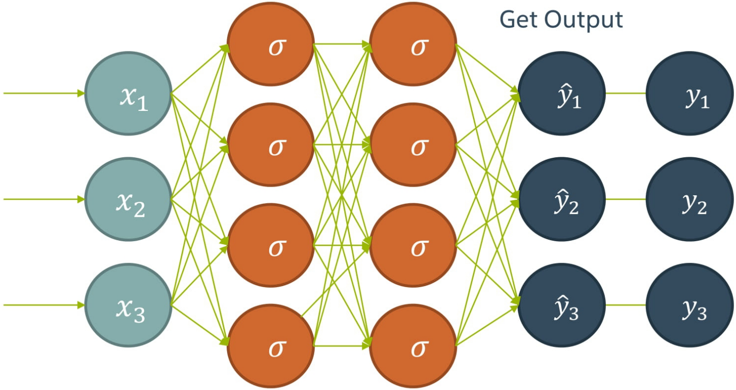
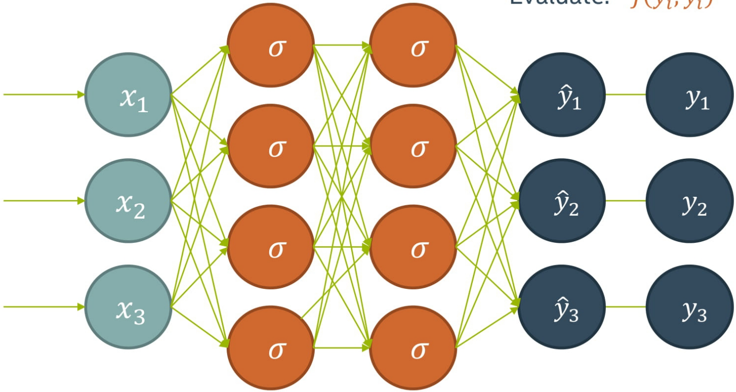


FORWARD PROPAGATION

Evaluate: $J(y_i, \hat{y}_i)$



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HOW TO CALCULATE GRADIENT?

Chain rule

Chain Rule Refresher

- Foward propagation can be viewed as a long series of nested equations.
- **Backpropagation** is merely an application the Chain Rule to find the Derivatives of cost with respect to any variable in the nested equation. **Ex.**

  What is $\frac{df}{dx}$?

$$f(x) = A(B(C(x)))$$

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  Ex.

  What is $\frac{df}{dx}$?

$$f(x) = A(B(C(x)))$$

$$\frac{df}{dx} = \frac{dA}{dB} * \frac{dB}{dC} * \frac{dC}{dx}$$

HOW TO TRAIN A NEURAL NET?

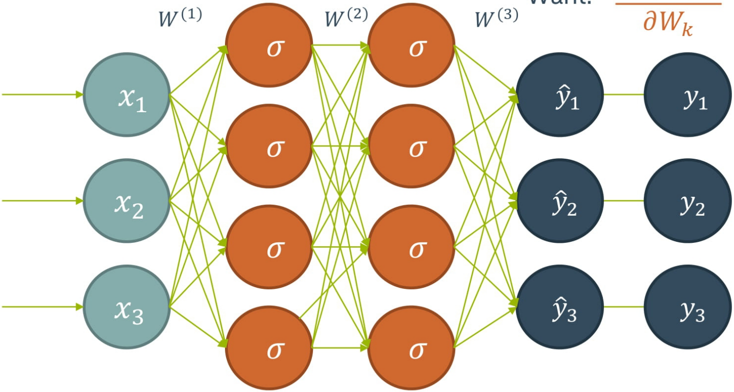
- How could we change the weights to make our Loss Function lower?
- Think of neural net as a function F: X -> Y
- F is a complex computation involving many weights W_k
- Given the structure, the weights “define” the function F (and therefore define our model)
- Loss Function is J(y,F(x))

HOW TO TRAIN A NEURAL NET?

- Get $\frac{\partial J}{\partial W_k}$ for every weight in the network.
- This tells us what direction to adjust each Wk if we want to lower our loss function.
- Make an adjustment and repeat!

FEEDFORWARD NEURAL NETWORK

Want: $\frac{\partial J(y_i, \hat{y}_i)}{\partial W_k}$



CALCULUS TO THE RESCUE

- Use calculus, chain rule, etc. etc.
- Functions are chosen to have "nice" derivatives
- Numerical issues to be considered

PUNCHLINE

$$\frac{\partial J}{\partial W^{(3)}} = (\hat{y} - y) \cdot a^{(3)}$$

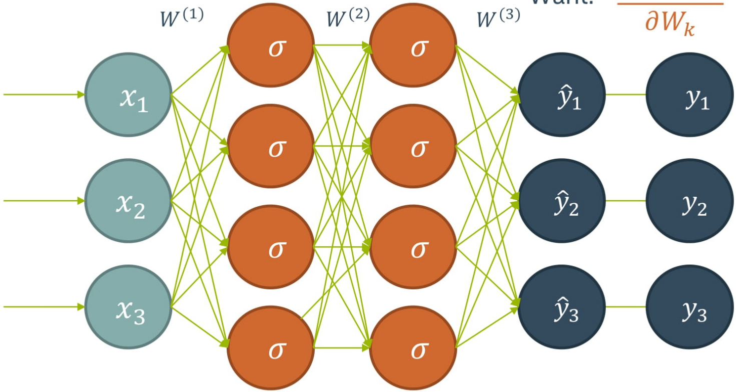
$$\frac{\partial J}{\partial W^{(2)}} = (\hat{y} - y) \cdot W^{(3)} \cdot \sigma'\left(z^{(3)}\right) \cdot a^{(2)}$$

$$\frac{\partial J}{\partial W^{(1)}} = (\hat{y} - y) \cdot W^{(3)} \cdot \sigma'\left(z^{(3)}\right) \cdot W^{(2)} \cdot \sigma'\left(z^{(2)}\right) \cdot X$$

- Recall that: $\sigma'(z) = \sigma(z)(1-\sigma(z))$
- Though they appear complex, above are easy to compute!

BACKPROPAGATION

Want: $\dfrac{\partial J(y_i, \hat{y}_i)}{\partial W_k}$



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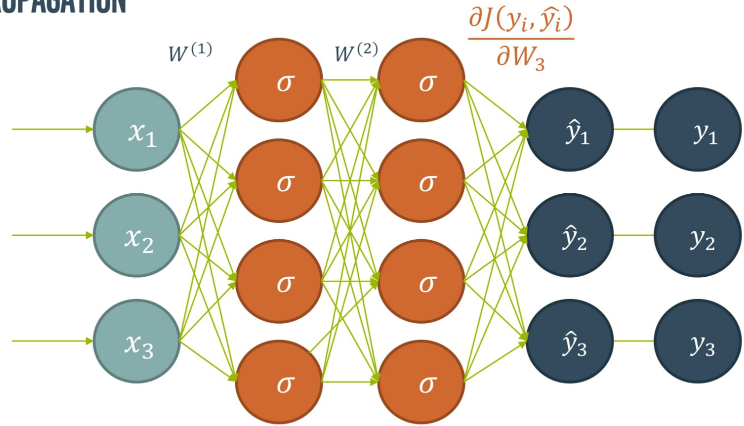

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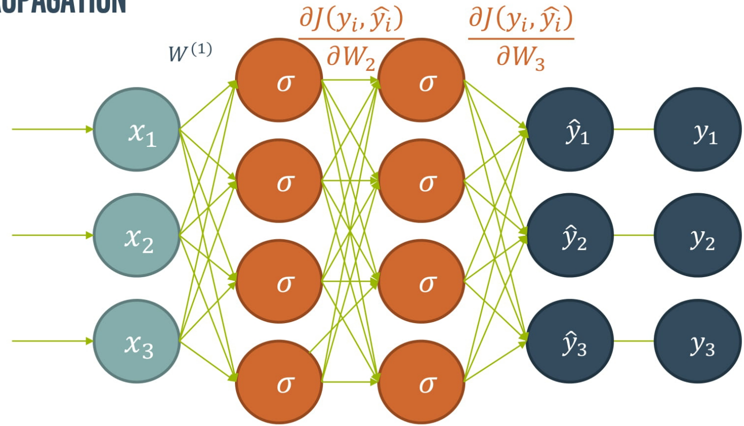

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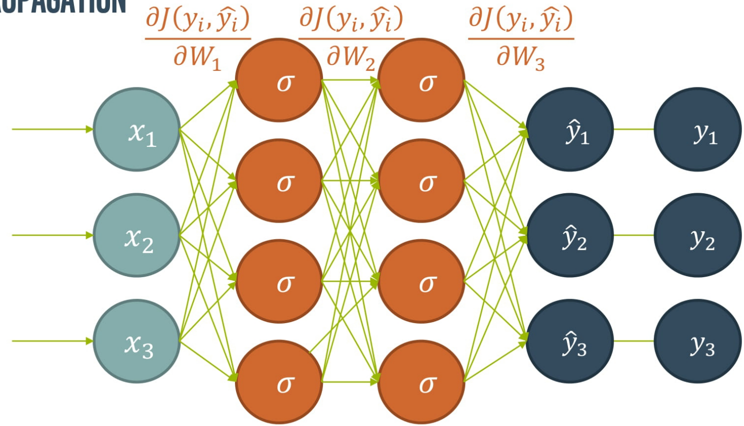

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VANISHING GRADIENTS

Recall that:

$$\frac{\partial J}{\partial W^{(1)}} = (\hat{y} - y) \cdot W^{(3)} \cdot \sigma'\left(z^{(3)}\right) \cdot W^{(2)} \cdot \sigma'\left(z^{(2)}\right) \cdot X$$

- Remember: $\sigma'(z) = \sigma(z)(1-\sigma(z)) \leq .25$
- As we have more layers, the gradient gets very small at the early layers.
- This is known as the “vanishing gradient” problem.
- For this reason, other activations (such as ReLU) have become more common.

WHAT NEXT?

- **Given an example (or group of examples), we know how to compute the derivative for each weight.**
- **How exactly do we update the weights?**
- **How often? (after each training data point? after all the training data points?)**

WHAT NEXT?—GRADIENT DESCENT

- W_new = W_old - lr * derivative
- Classical approach—get derivative for entire data set, then take a step in that direction
- Pros: Each step is informed by all the data
- Cons: Very slow, especially as data gets big

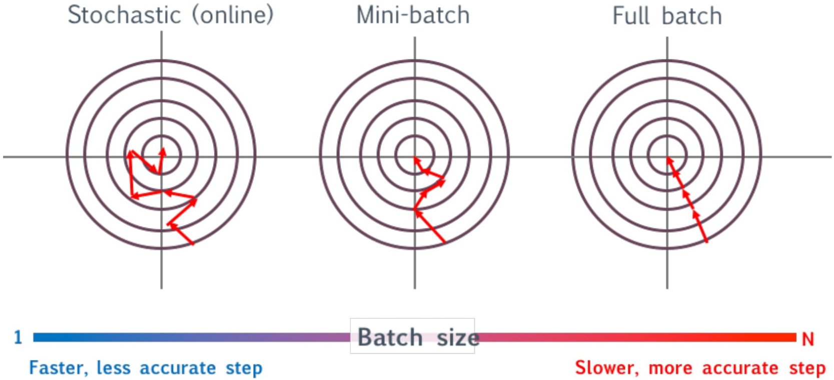
ANOTHER APPROACH: STOCHASTIC GRADIENT DESCENT

- Get derivative for just one point, and take a step in that direction
- Steps are “less informed” but you take more of them
- Should “balance out”
- Probably want a smaller step size
- Also helps “regularize”

COMPROMISE APPROACH: MINI-BATCH

- Get derivative for a "small" set of points, then take a step in that direction
- Typical mini batch sizes are 16, 32
- Strikes a balance between two extremes

COMPARISON OF BATCHING APPROACHES



BATCHING TERMINOLOGY

Full-batch:
Use entire data set to compute gradient before updating

Mini-batch:
Use a smaller portion of data (but more than single example) to compute gradient before updating

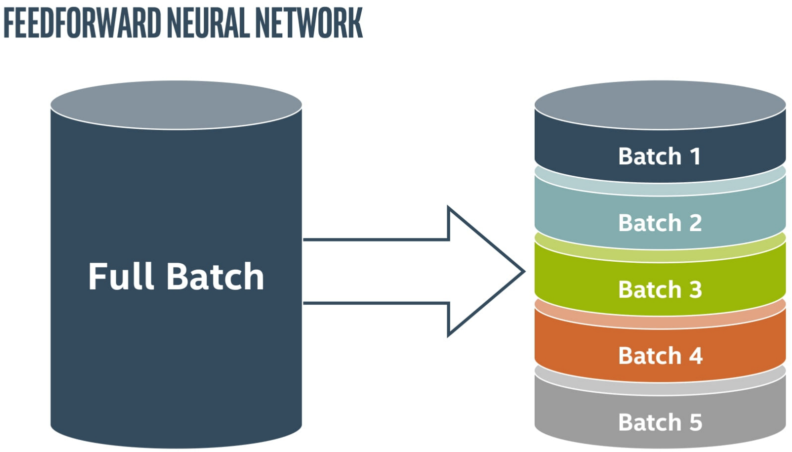
Stochastic Gradient Descent (SGD):
Use a single example to compute gradient before updating (though sometimes people use SGD to refer to minibatch, also)

BATCHING TERMINOLOGY

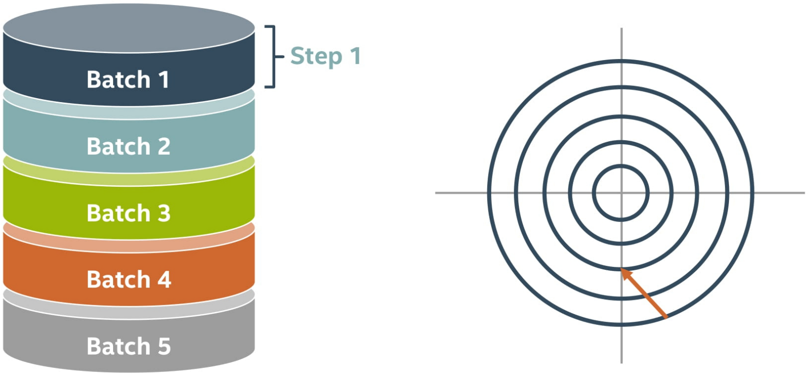
- An **Epoch** refers to a single pass through all of the training data.
- In full batch gradient descent, there would be one step taken per epoch.
- In SGD / Online learning, there would be n steps taken per epoch (n = training set size)
- In Minibatch there would be (n/batch size) steps taken per epoch
- When training, it is common to refer to the number of epochs needed for the model to be "trained".

NOTE ON DATA SHUFFLING

- **To avoid any cyclical movement and aid convergence, it is recommended to shuffle the data after each epoch.**
- **This way, the data is not seen in the same order every time, and the batches are not the exact same ones.**


FEEDFORWARD NEURAL NETWORK
Full Batch
Batch 1
Batch 2
Batch 3
Batch 4
Batch 5

TRAINING IN ACTION



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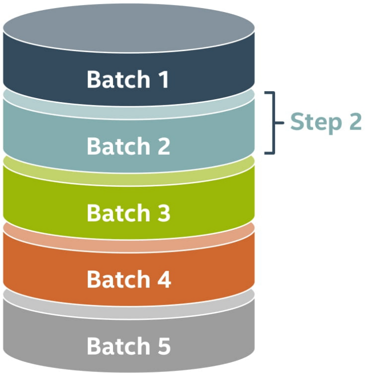

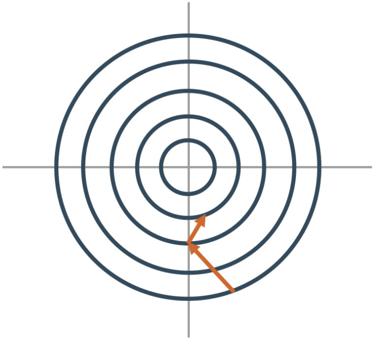

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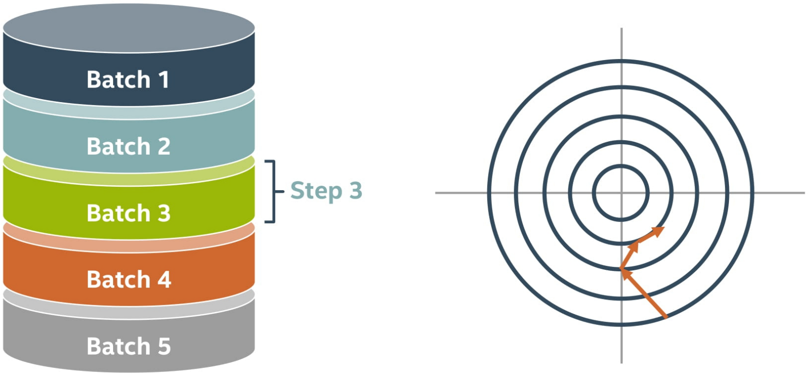

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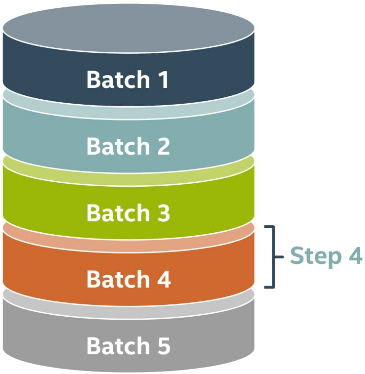

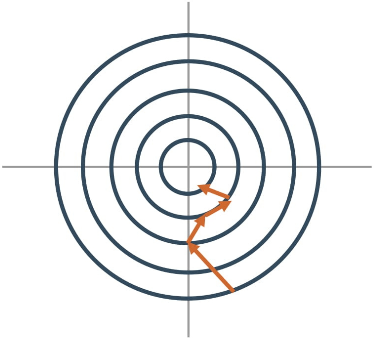

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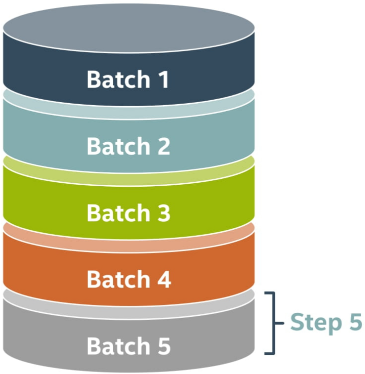
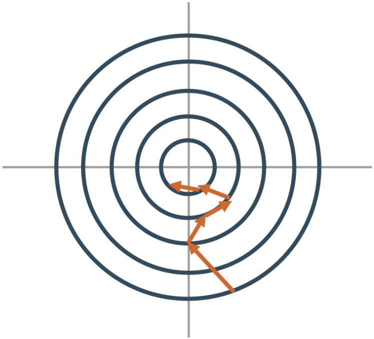
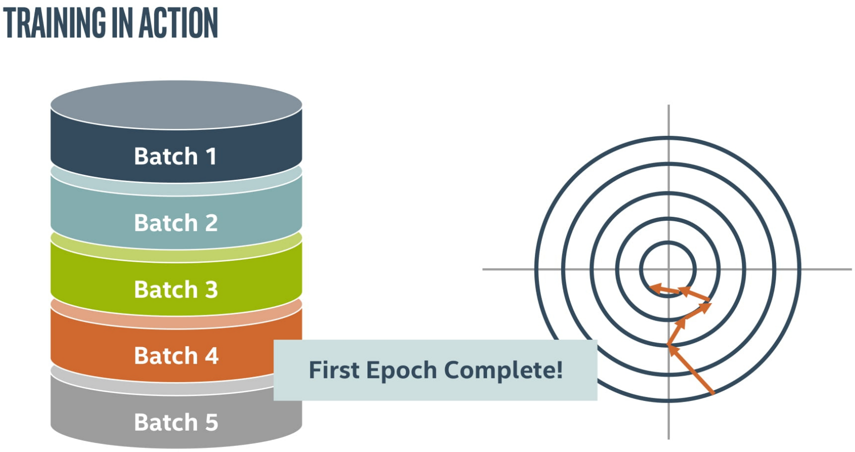
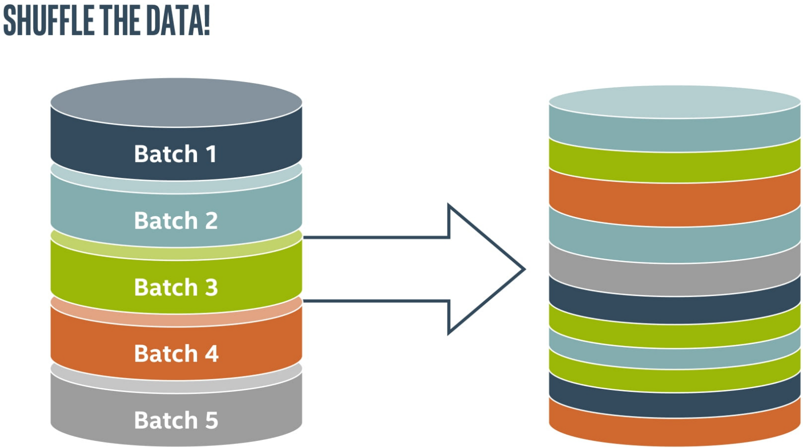





TRAINING IN ACTION
Batch 1
Batch 2
Batch 3
Batch 4
Batch 5
First Epoch Complete!


SHUFFLE THE DATA!
Batch 1
Batch 2
Batch 3
Batch 4
Batch 5

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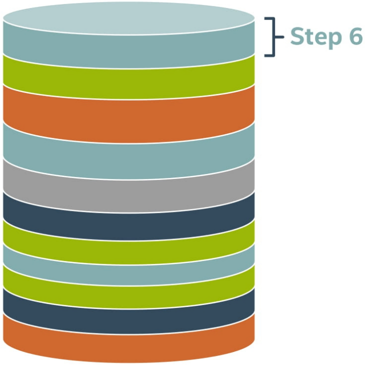
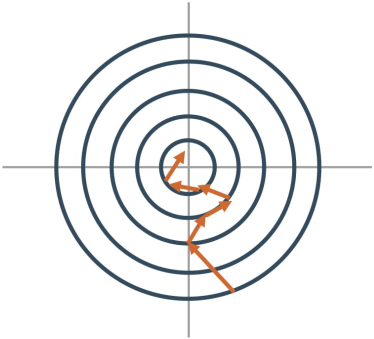




THE KERAS PACKAGE

- Keras allows easy construction, training, and execution of Deep Neural Networks
- Written in Python, and allows users to configure complicated models directly in Python
- Uses either Tensorflow or Theano “under the hood”
- Uses either CPU or GPU for computation
- Uses numpy data structures, and a similar command structure to scikit-learn (model.fit , model.predict, etc.)

TYPICAL COMMAND STRUCTURE IN KERAS

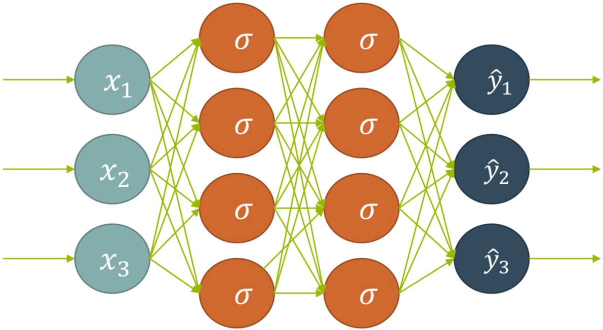
- **Build the structure of your network.**
- **Compile the model, specifying your loss function, metrics, and optimizer (which includes the learning rate).**
- **Fit the model on your training data (specifying batch size, number of epochs)**
- **Predict on new data**
- **Evaluate your results**

BUILDING THE MODEL

- Keras provides two approaches to building the structure of your model:
- Sequential Model: allows a linear stack of layers – simpler and more convenient if model has this form
- Functional API: more detailed and complex, but allows more complicated architectures
- We will focus on the Sequential Model.

RUNNING EXAMPLE, THIS TIME IN KERAS

Let's build this Neural Network structure shown below in Keras:



KERAS—SEQUENTIAL MODEL

First, import the Sequential function and initialize your model object:

```
from keras.models import Sequential
model = Sequential()
```

KERAS—SEQUENTIAL MODEL

Then we add layers to the model one by one.

```
from keras.layers import Dense, Activation

# For the first layer, specify the input dimension
model.add(Dense(units=4, input_dim=3))

# Specify an activation function
model.add(Activation(sigmoid'))

# For subsequent layers, the input dimension is presumed from
# the previous layer
model.add(Dense(units=4))
model.add(Activation(sigmoid'))
model.add(Dense(units=3))
model.add(Activation('softmax'))
```

MULTICLASS CLASSIFICATION WITH NEURAL NETWORKS

- **For binary classification problems, we have a final layer with a single node and a sigmoid activation.**
- **This has many desirable properties**
  - Gives an output strictly between 0 and 1
  - Can be interpreted as a probability
  - Derivative is “nice”
  - Analogous to logistic regression
- **Is there a natural extension of this to a multiclass setting?**

MULTICLASS CLASSIFICATION WITH NEURAL NETWORKS

- Reminder: one hot encoding for categories
- Take a vector with length equal to the number of categories
- Represent each category with one at a particular position (and zero everywhere else)

$$\begin{array}{ccc} \begin{bmatrix}1\\0\\0\end{bmatrix} & \begin{bmatrix}0\\1\\0\end{bmatrix} & \begin{bmatrix}0\\0\\1\end{bmatrix} \\ \textbf{Cat} & \textbf{Dog} & \textbf{Toaster} \end{array}$$

MULTICLASS CLASSIFICATION WITH NEURAL NETWORKS

- **For multiclass classification problems, let the final layer be a vector with length equal to the number of possible classes.**
- **Extension of sigmoid to multiclass is the softmax function.**
- $softmax(z_i) = \frac{e^{z_i}}{\sum_{k=1}^{K} e^{z_k}}$
- **Yields a vector with entries that are between 0 and 1, and sum to 1**

MULTICLASS CLASSIFICATION WITH NEURAL NETWORKS

- For loss function use "categorical cross entropy"
- This is just the log-loss function in disguise

$$C.E. = -\sum_{i=1}^{n} y_i \log(\hat{y}_i)$$

- Derivative has a nice property when used with softmax

$$\frac{\partial C.E.}{\partial softmax} \cdot \frac{\partial softmax}{\partial z_i} = \hat{y}_i - y_i$$

WAYS TO SCALE INPUTS

- **Linear scaling to the interval [0,1]**

$$x_i = \frac{x_i - x_{min}}{x_{max} - x_{min}}$$

- **Linear scaling to the interval [-1,1]**

$$x_i = 2\left(\frac{x_i - \bar{x}}{x_{max} - x_{min}}\right) - 1$$

WAYS TO SCALE INPUTS

- **Standardization (making variable approx. std. normal)**

$$x_i = \frac{x_i - \bar{x}}{\sigma}; \qquad \sigma = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})^2}$$

Deep Learning Frameworks (1/2)

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- Sonnet

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- Sonnet
  - Built on top of TensorFlow.

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  - Built on top of TensorFlow.
  - High-level object-oriented libraries.

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  - Enables models to be trained in one framework and transferred to another for inference.

References

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Questions